INFORMATION TOPOLOGY

WHAT IS A MANIFOLD?

- A manifold is a kind of topological space.
  - No sense of distance or angles
  - Manifold vs. Manifold with boundary vs. Manifold with corner and different topological spaces
- Adding a metric to the manifold induces a topology, but adds additional structure (distance).
- MBAM does not operate on the geometric object.
  - MBAM uses the geometry, to find a topological feature: the boundary.

TO ILLUSTRATE

Consider the question:

What is the FIM for the enzyme-substrate model?

$$\frac{d}{dt}[E] = -k_f[E][S] + k_r[C] + k_c[C]$$

$$\frac{d}{dt}[S] = -k_f[E][S] + k_r[C]$$

$$\frac{d}{dt}[C] = k_f[E][S] - k_r[C] - k_c[C]$$

$$\frac{d}{dt}[P] = k_c[C]$$

This question makes no sense.

ON THE OTHER HAND

What are the boundaries of the enzyme-substrate model?:

$$\frac{d}{dt}[E] = -k_f[E][S] + k_r[C] + k_c[C]$$

$$\frac{d}{dt}[S] = -k_f[E][S] + k_r[C]$$

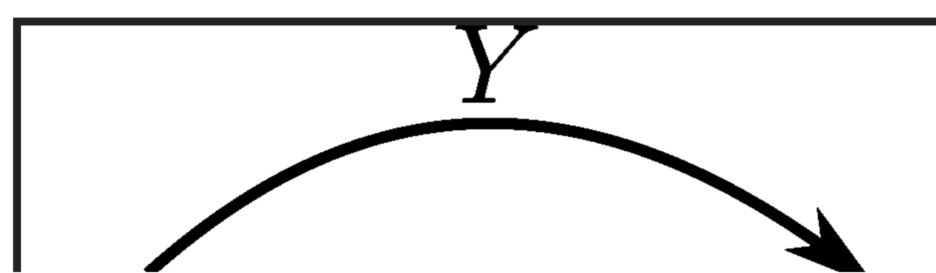
$$\frac{d}{dt}[C] = k_f[E][S] - k_r[C] - k_c[C]$$

$$\frac{d}{dt}[P] = k_c[C]$$

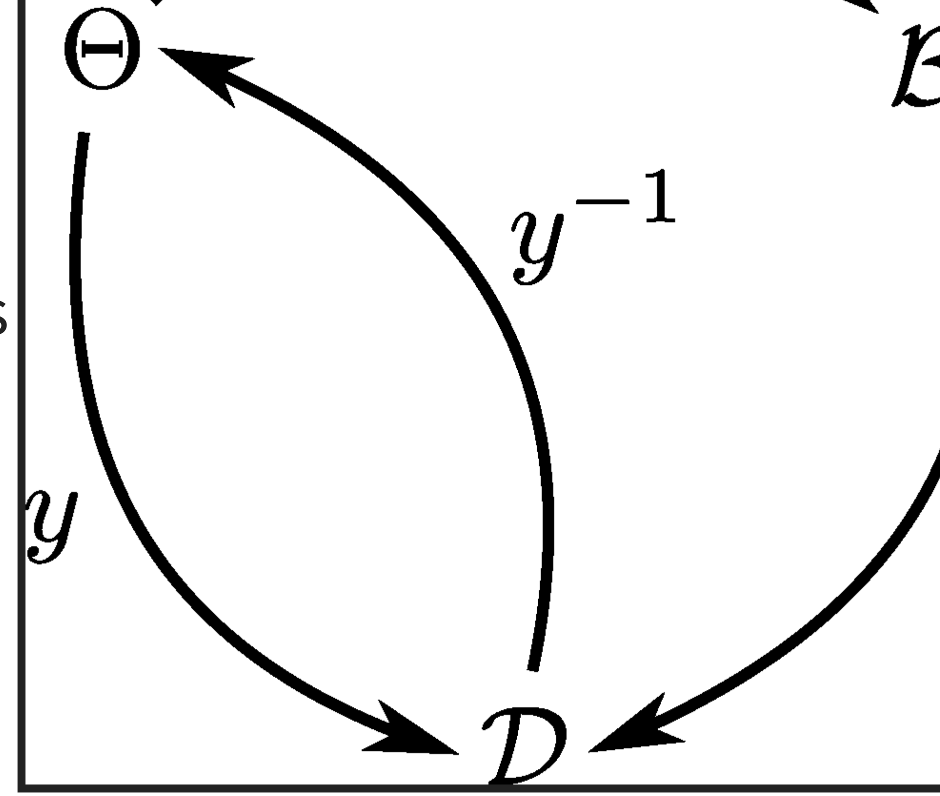
This question is well-posed.

The equilibrium approximation (Michaelis-Menten reaction) is one of the boundaries of this model.

MODELING

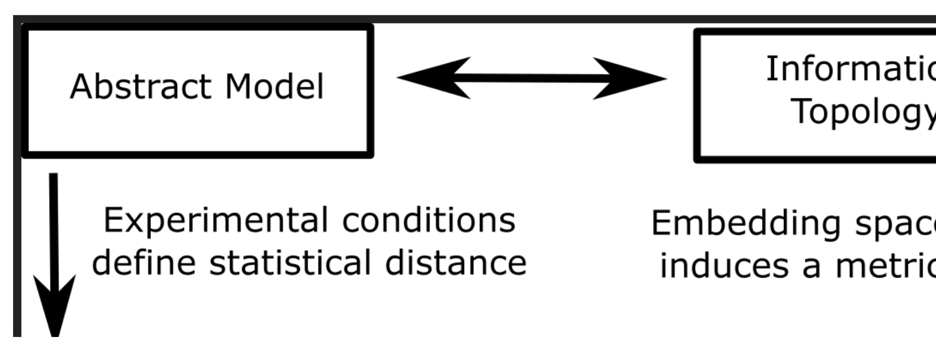


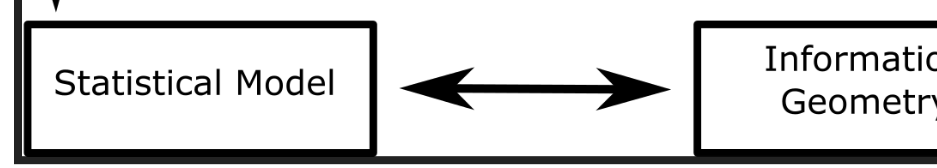
- Θ: Parameter Space
- Y: Model mapping
- $\mathcal{B}$: Behavior Space
  - All possible behaviors/measurements (large)
  - Induced by the mapping from parameter space Y.
- X: A real experiment
- $\mathcal{D}$: Data space induced by X.
- y: The model mapping from parameter space to data space.
  - What we have studied so far.
- y^{-1}: Parameter Inference from experimental data.



Transtrum, Mark K., Gus Hart, and Peng Qiu. "Information topology identifies emergent model classes." arXiv preprint arXiv:1409.6203 (2014).

STATISTICAL VS. ABSTRACT MODELS



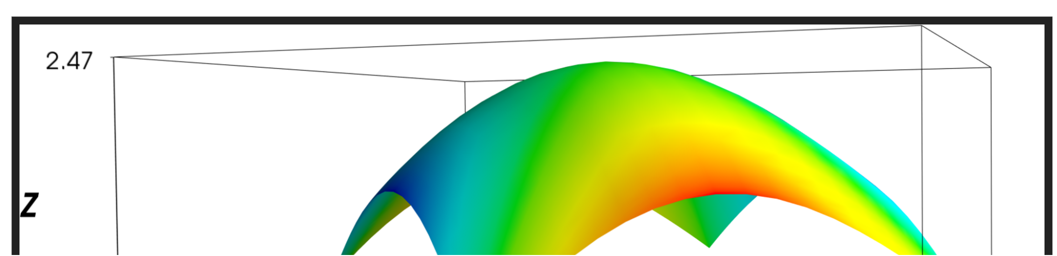


- Parameter space and potential behaviors exist independently of real experiments.
  - No natural metric.
  - Manifold in the topological sense.
- Statistical inference on real data adds a metric to the manifold.
  - Natural Metric
  - Manifold in the geometric sense.

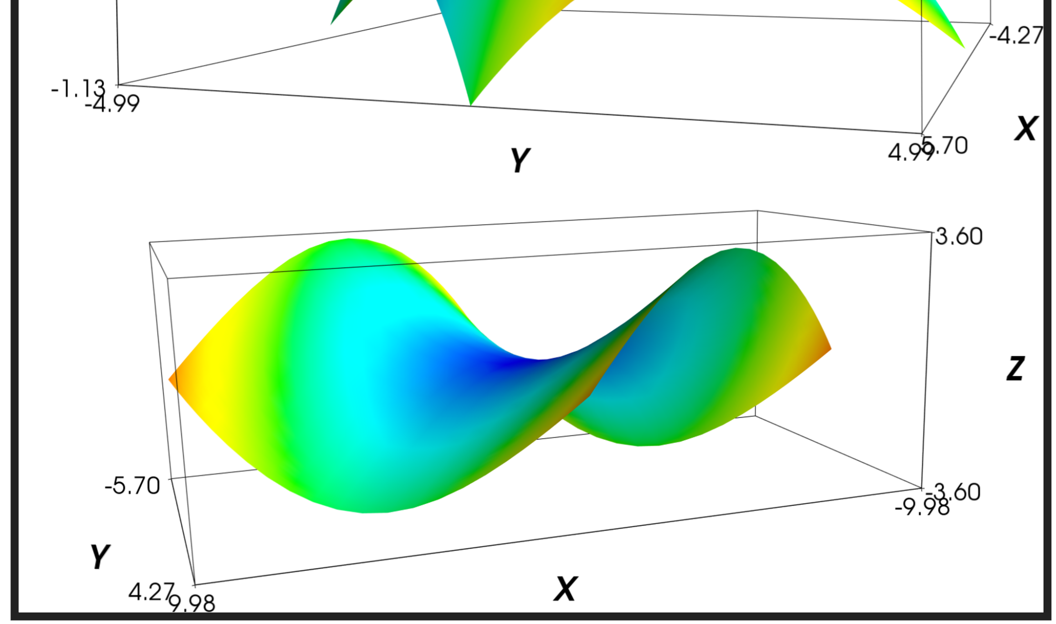
- Statistical Model: a model for which the Fisher Information *is* defined.
  - Requires data/predictions
  - Information Geometry
- Abstract Model: A parameter space and model mapping for which potential Fisher Informations *could be* defined.
  - Information Topology

EXAMPLE:

$$y_1 = e^{-\theta_1 t} + e^{-\theta_2 t}$$
$$y_2 = e^{-\theta_1 t} - e^{-\theta_2 t}$$



- Different measurements of y_1 and y_2 can lead to different geometries (e.g., curvatures).
- In either case, the boundary complex is the same (i.e., square like)
- The "square-likeness" is a property of the abstract model
- We say the manifold is a "topological square"



TOPOLOGY

Information Topology: Study of the boundary complex of the abstract model compared to the boundary structure of the statistical model induced by the Fisher Information Matrix.

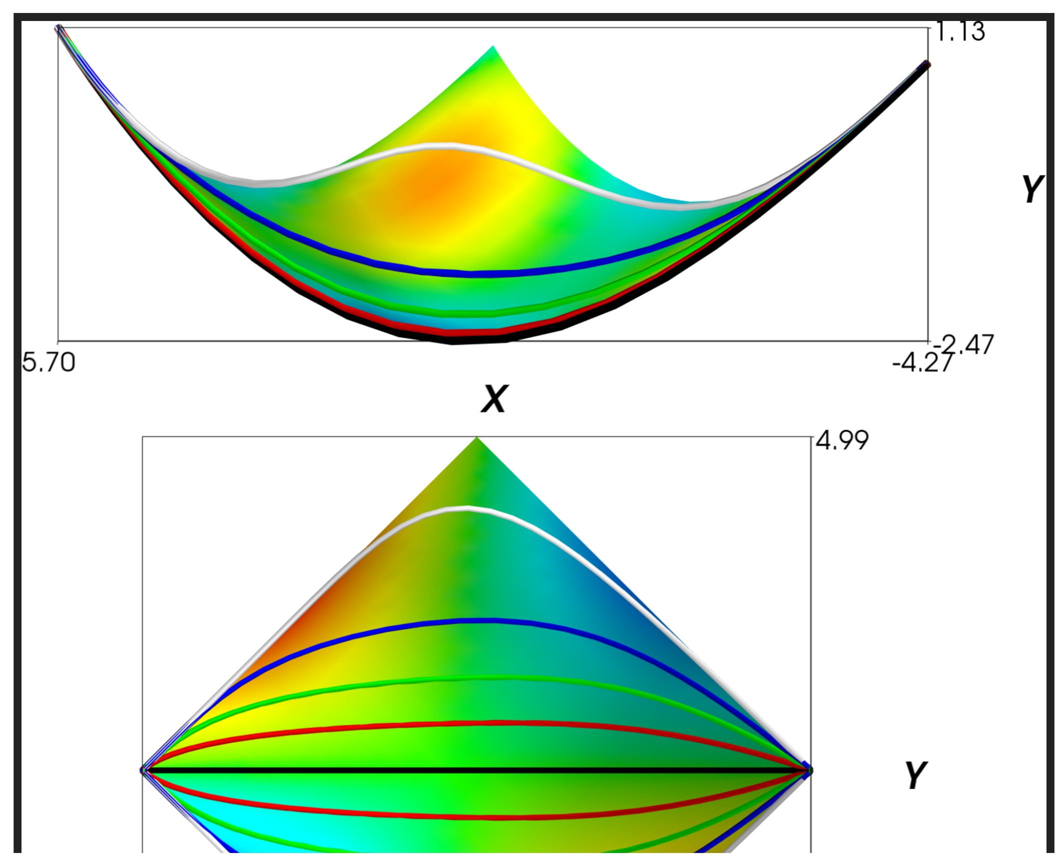
MANIFOLD COLLAPSE

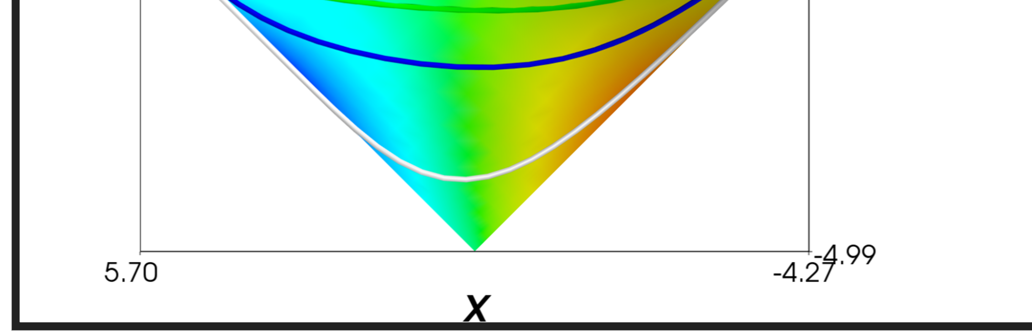
- Non-standard (Not counting "holes" in the manifold, although that could be done.)
- This analysis is topological in several ways:
  - Global (not local)
  - Invariance to classes of transformations (diffeomorphisms rather than homeomorphisms)
  - Studies properties of a topological space (in most cases, abstract models are CW complexes)
  - Related to the origin of topology (Euler's polyhedra formula)
  - Is independent of the Fisher Information Matrix.

- The Fisher Information Metric *induces* a topology on the parameter space.
- This topology need not be the same as that of the abstract model.
- When the FIM topology is different from the abstract topology, we say there was *Manifold Collapse*.

EXAMPLE:

$$y_1 = e^{-\theta_1 t} + e^{-\theta_2 t}$$
$$y_2 = e^{-\theta_1 t} - e^{-\theta_2 t}$$

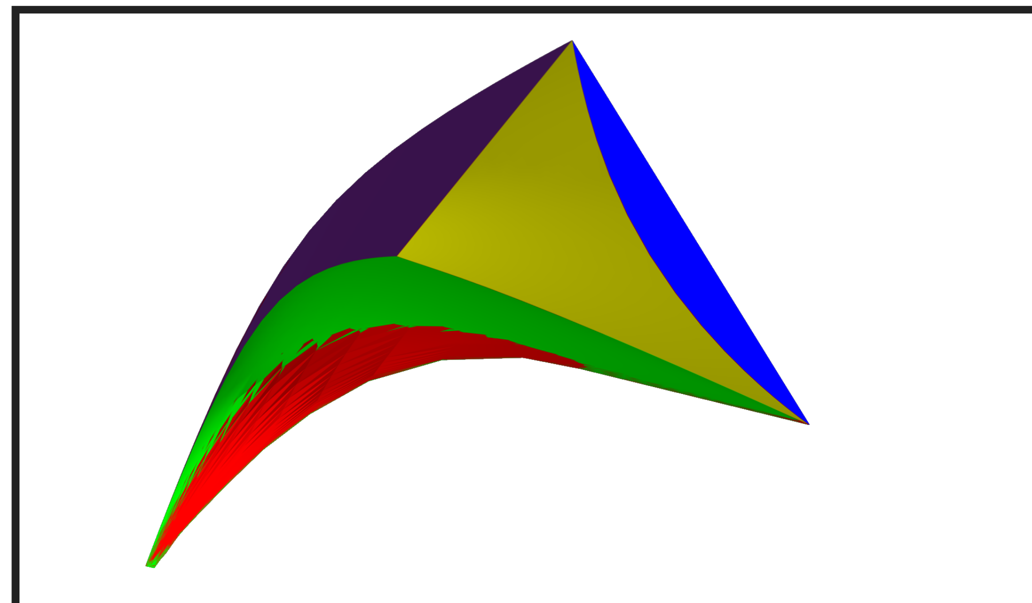


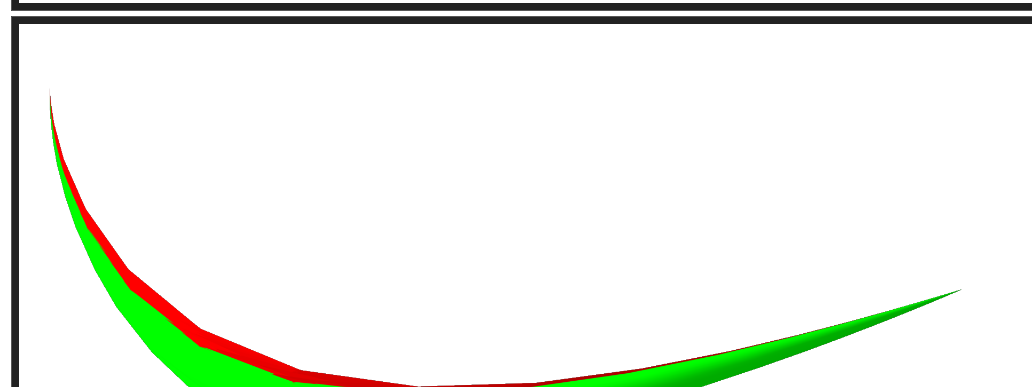


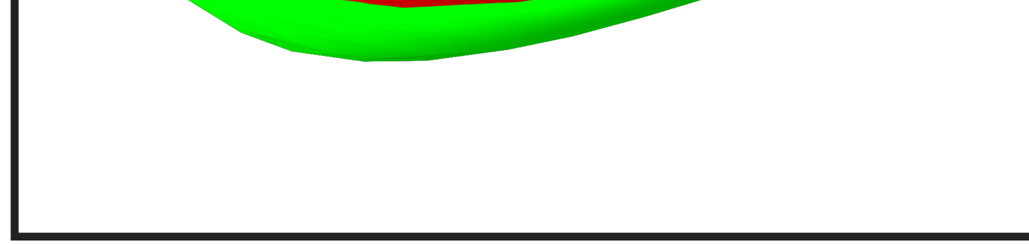
- But suppose I only observe y_1.
- The manifold is "folded" in half.
- It is now "triangle-like".

COLLAPSE OF THE BOUNDARIES

- The collapse reflects a qualitative change in the information content of the data and results in a structural nonidentifiability.



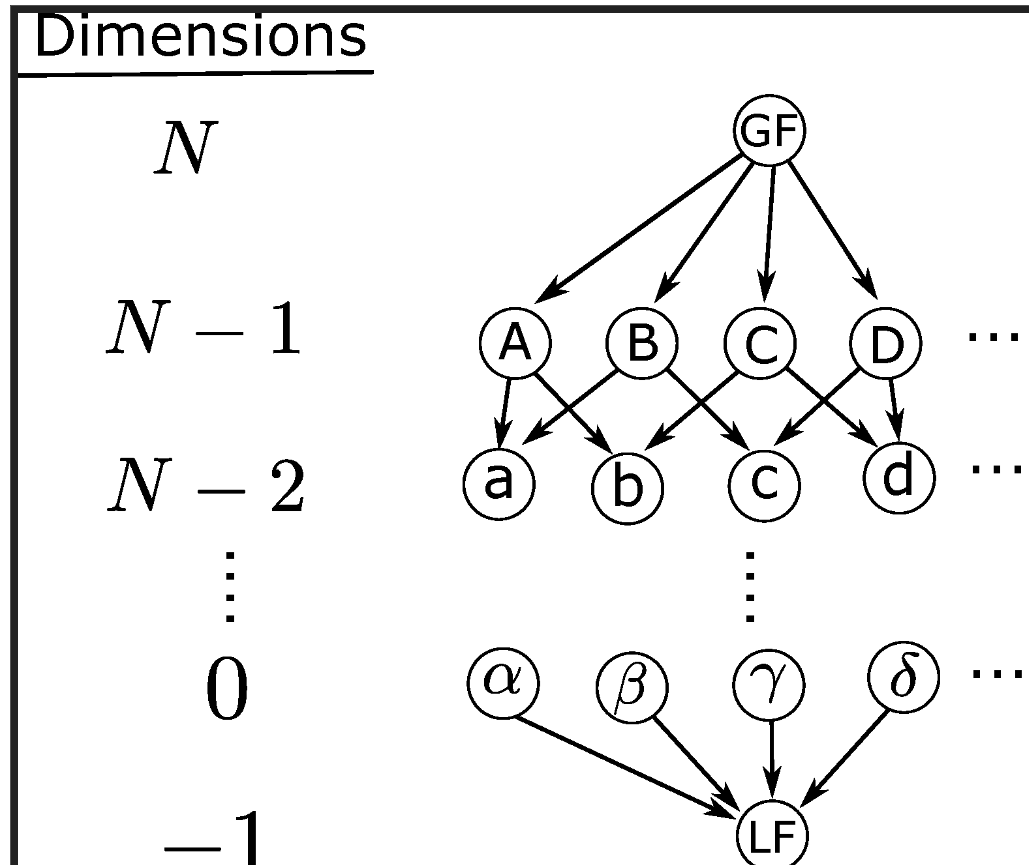




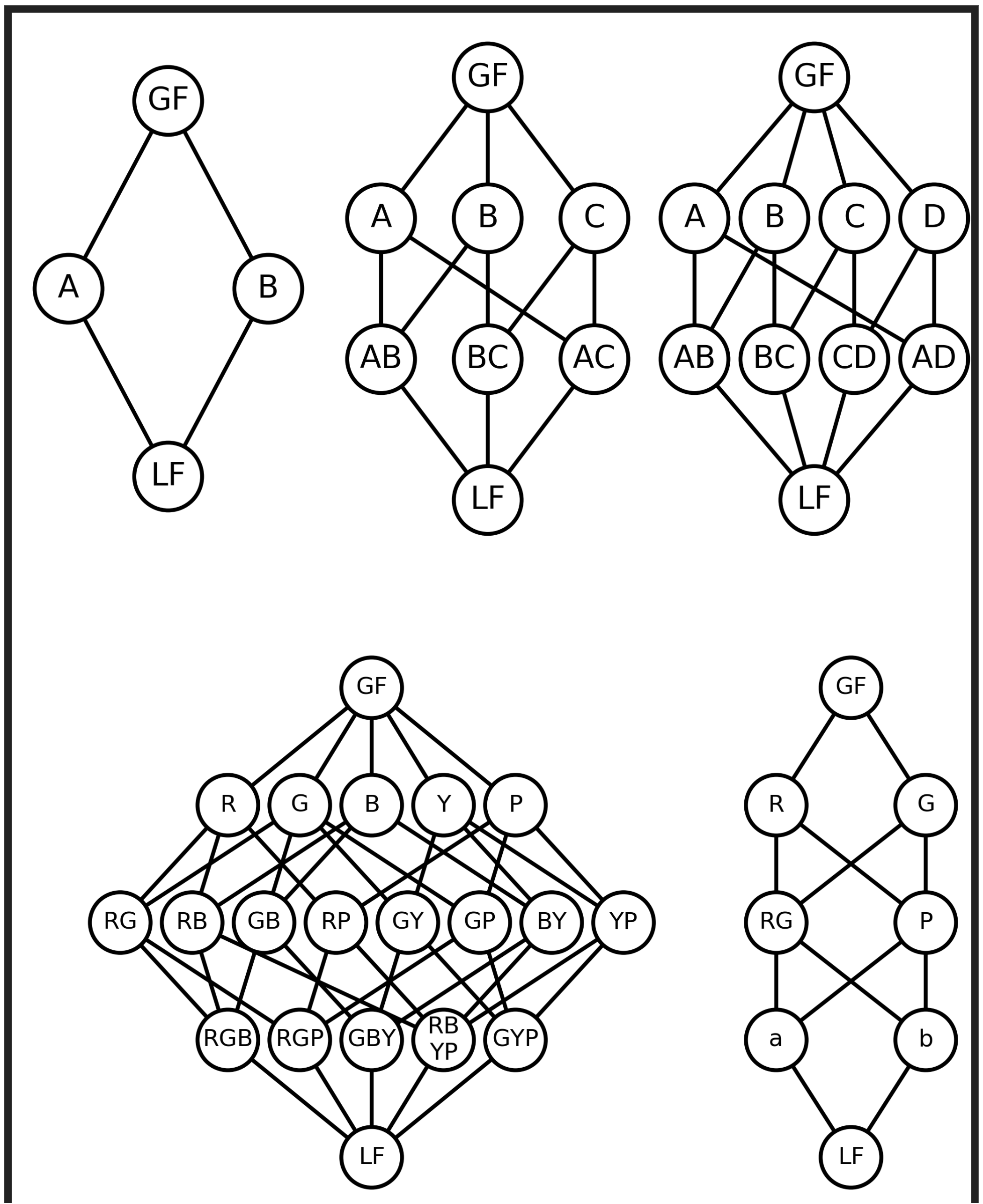
- Sometimes the boundary structure changes without a structural nonidentifiability.
- The abstract enzyme-substrate model is three dimensional with five faces.
- The statistical enzyme-substrate model when observing only the product $[P]$ is three dimensional with two faces.
- The boundary collapse leads to a practical nonidentifiability.
- The success of the Michaelis-Menten approximation is a consequence of this boundary collapse.

HASSE DIAGRAMS

- The hierarchy of boundaries forms a graded partially ordered set (poset)
- Posets are graphically represented by Hasse diagrams.
- Nodes represent boundary structures.
  - Rows indicate dimension.
  - Arrows indicate adjacency relationships.
- It is customary to include a single "Least Face" (LF) corresponding to dimension -1.



EXAMPLES



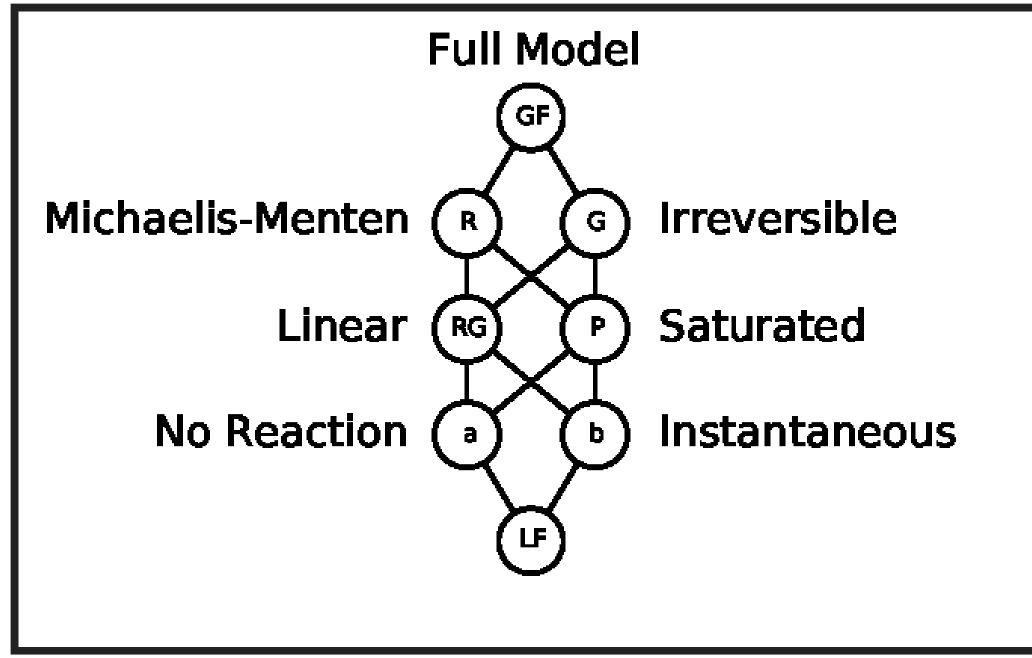
Hasse Diagrams for:

- Line Segment
- Triangle
- Square
- Abstract enzyme-substrate model
- Statistical enzyme-substrate model

MEANING OF NODES

Nodes in the Hasse diagram:

- Simplified Models
- Approximate a portion of the abstract model.
- Distinct Behavioral regimes



The Hasse diagram is a road map from the intricate and fully parameterized description of a complex system through various types of approximations to the set of distinct behavior regimes the model enables.

MANIFOLD COLLAPSE REVISITED

- A statistical manifold has a topology (boundary complex) induced by the metric.
- This boundary complex may or may not be the same as that of the abstract model.
- Families of statistical models with the same boundary complex are related by diffeomorphisms.
  - Result of differential topology: Diffeomorphisms form a group.
  - Groups of statistical models with the same Hasse diagram.

OBSERVATION SEMI-GROUP

- When the manifold "collapses" information is lost--the operation has no inverse.
  - The group structure relating statistical manifolds is broken.
- The collection of all possible statistical manifolds forms a semi-group. (Like a group, but with no inverse.)
- Within the semi-group are proper subgroups of statistical manifolds characterized by their common Hasse diagram.
- There is a partial ordering of these subgroups.
  Let G_1 and G_2 are two sub-groups. If there exist statistical manifolds $\mathcal{M}_1 \in G_1$ and $\mathcal{M}_2 \in G_2$ such that the observations for $\mathcal{M}_1 \subset \mathcal{M}_2$ then $G_1 \prec G_2$

THE OBSERVATION SEMI-GROUP

Very little is known about the observation semi-group and the relationship among its subgroups.

- There exists a maximal subgroup G_{max}
- It's Hasse diagram is that of the abstract model.
- We speculate that parameter nonidentifiability (both structural and practical) can be defined in terms of the observation subgroups.

ABSTRACT MODEL MANIFOLD

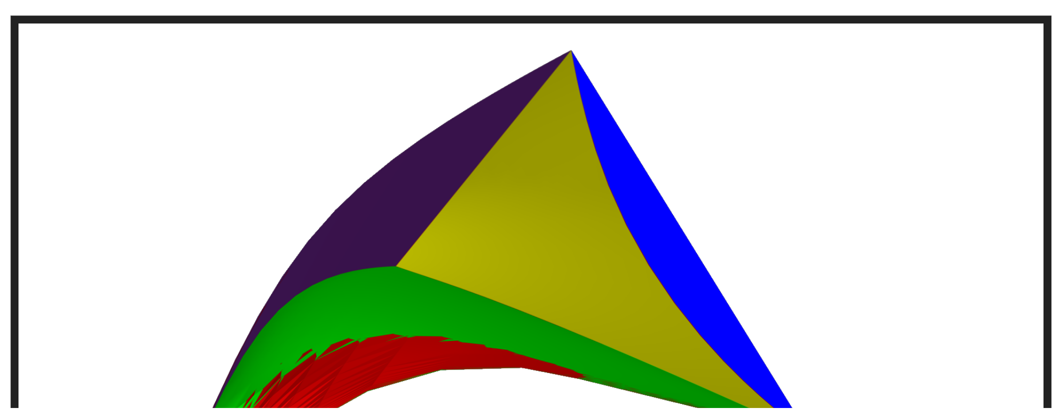
Many statistical manifolds have a common structure:

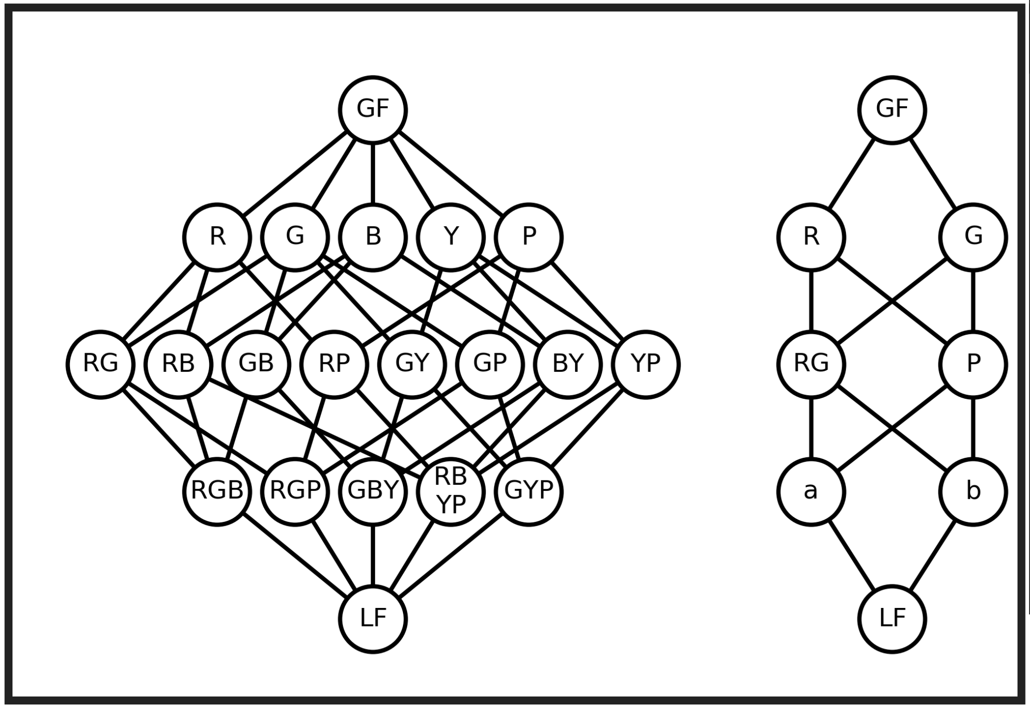
- A few long directions
- Many narrow directions
- Hyper-ribbon, low effective dimensionality
- Universality, effective theories, sloppiness

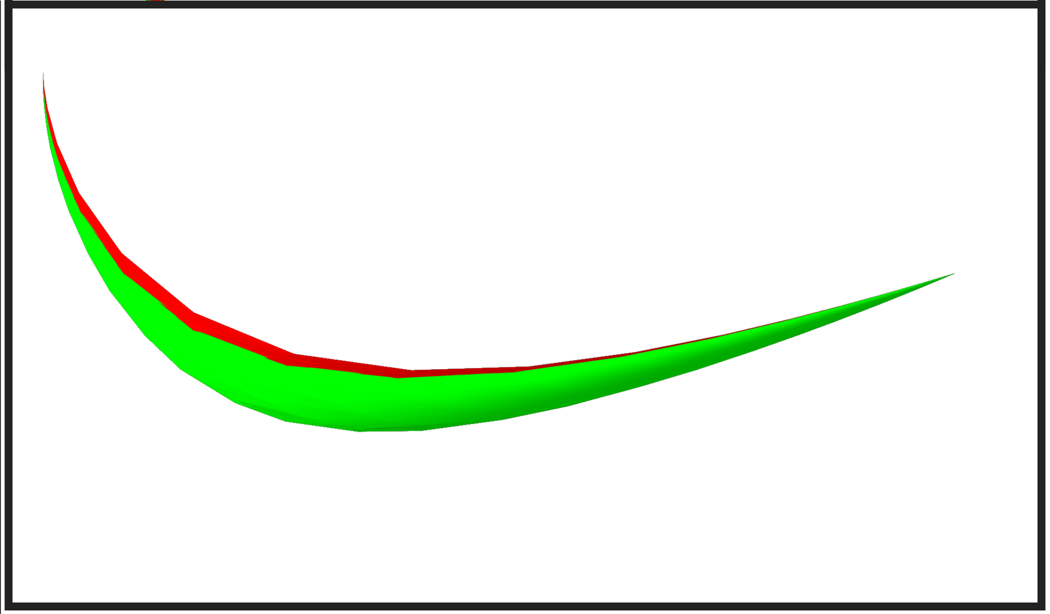
What is the structure of a typical abstract model manifold?

ABSTRACT MODEL MANIFOLD

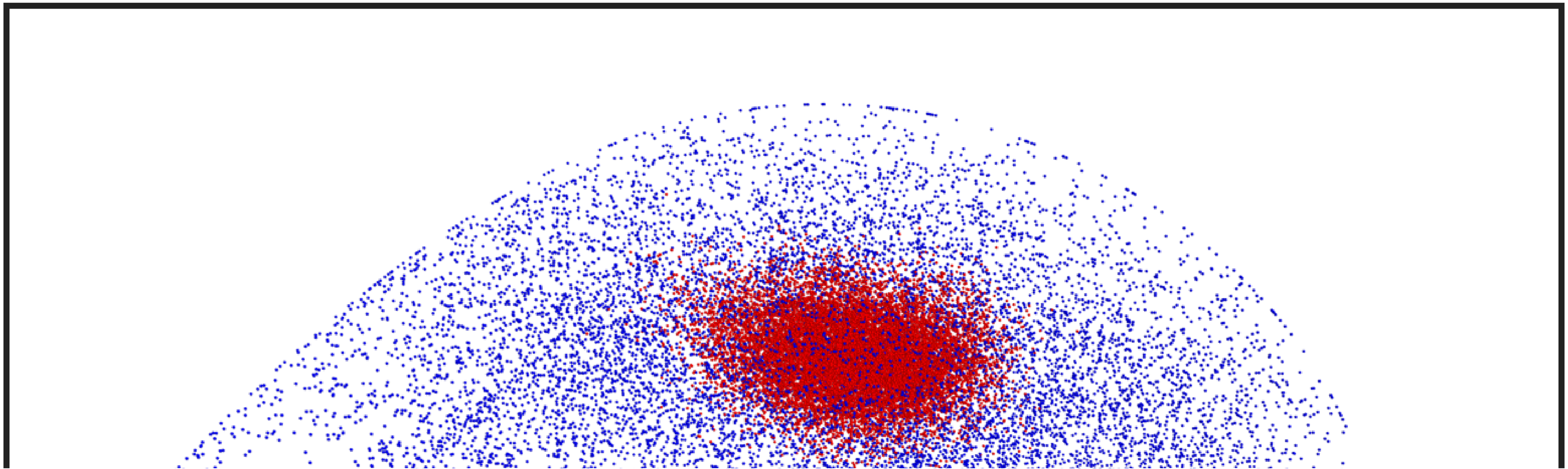
For a complex system, the Hasse diagram of the abstract manifold is combinatorially complex:

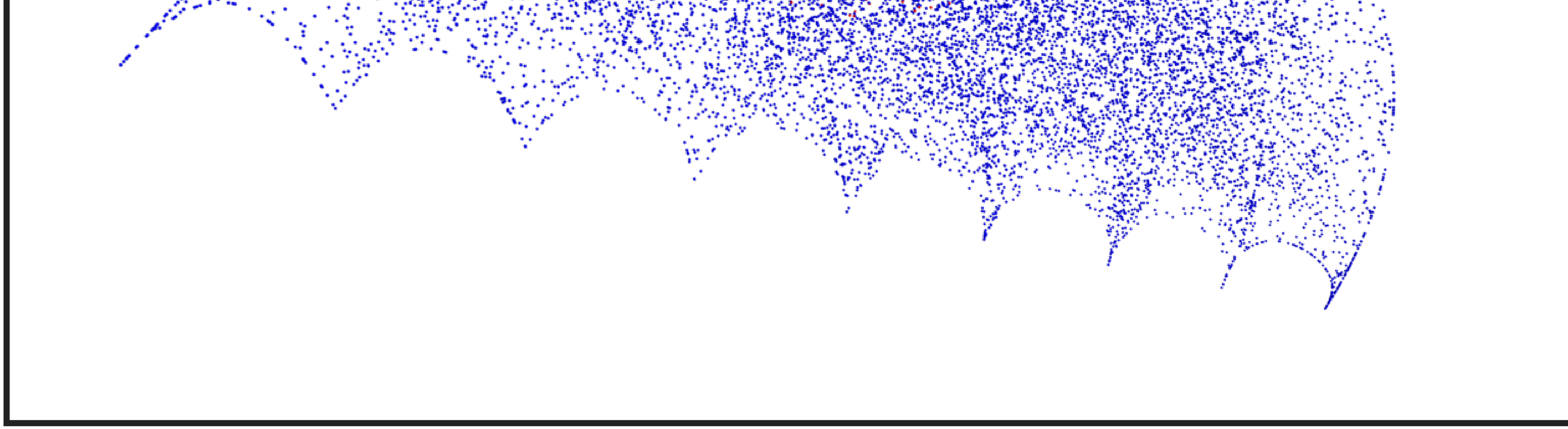




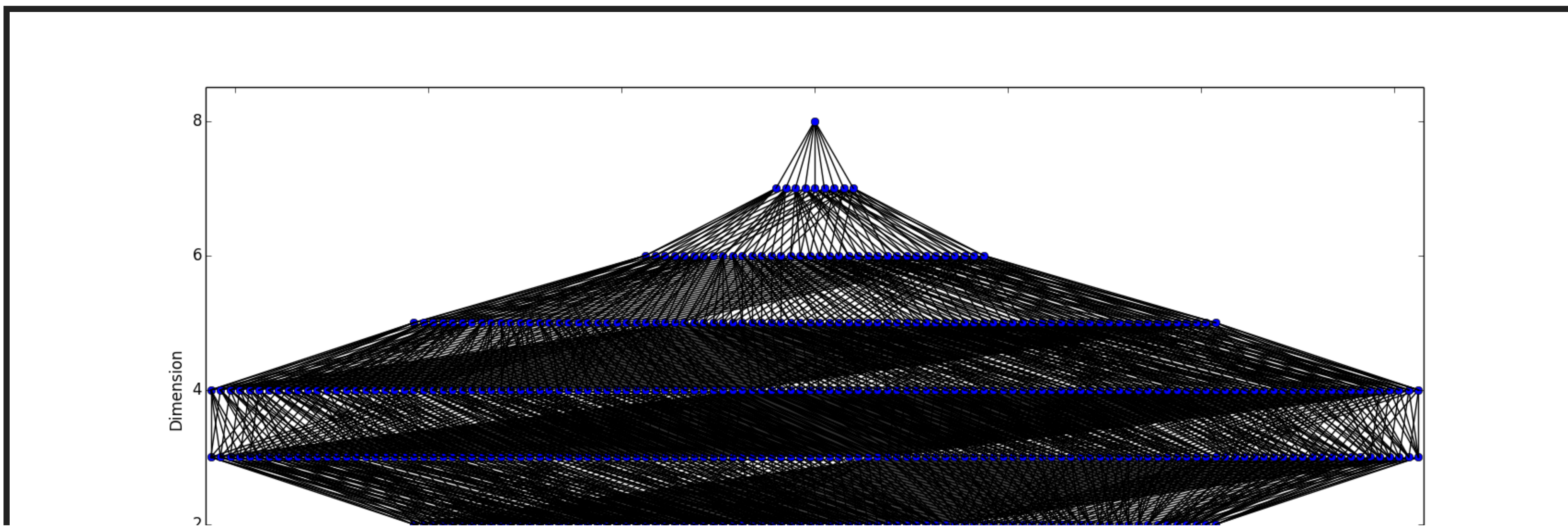


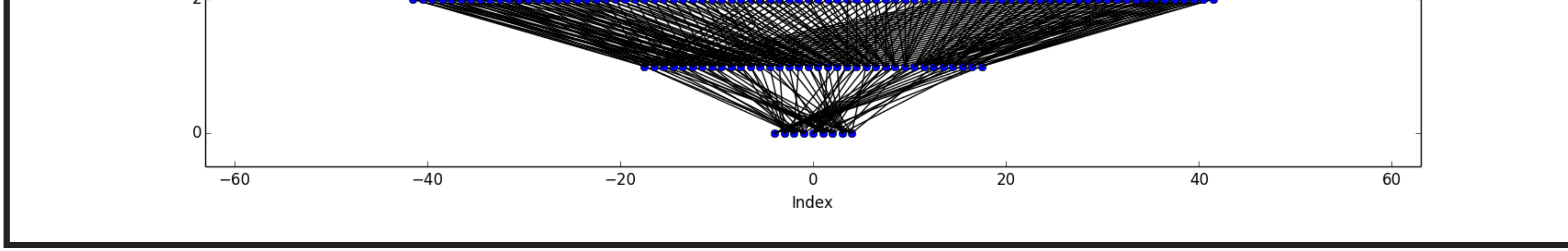
EXAMPLE: MULTIPLE EXPONENTIALS





EXAMPLE: CLUSTER EXPANSION





EXAMPLE: EXPONENTIAL FAMILIES

Probability distribution for a discrete set of outcomes:

$$P_i = \frac{1}{Z} e^{-\sum_\mu \Pi_{i\mu} \theta^\mu}$$

Completely characterized by the Π matrix.

- M outcomes
- N parameters

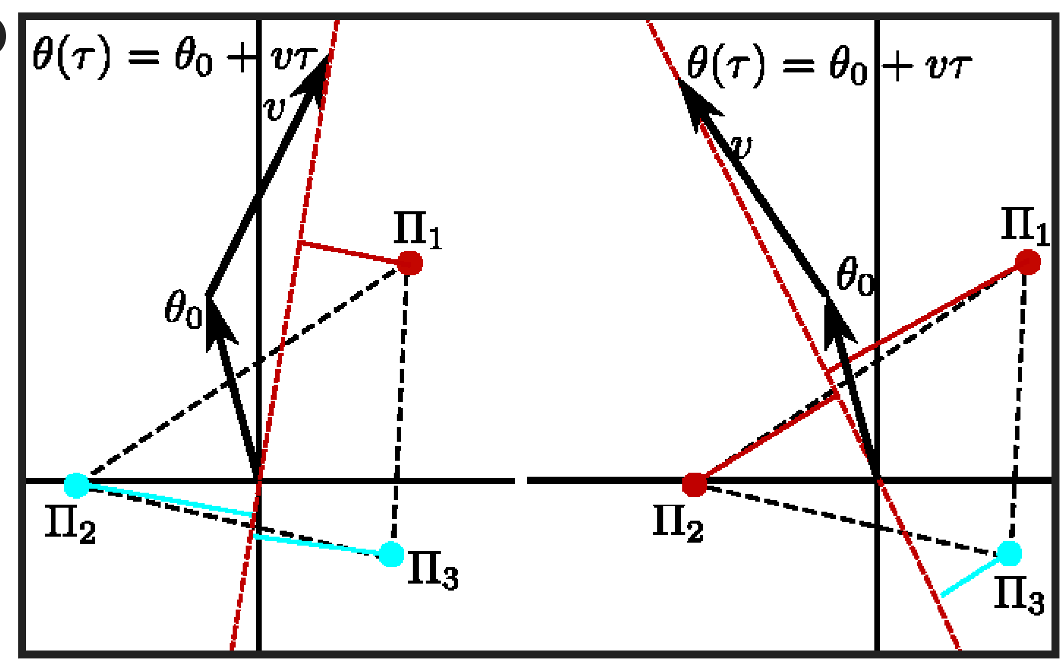
Π is an MxN matrix

Examples:

- Ising Model
- Markov Random Field
- Cluster Expansion (alloys crystal structure)

TOPOLOGY OF EXPONENTIAL FAMILIES

- Each row of Π corresponds to a particular outcome (e.g., crystal structure)
- Each row of Π is a vector in parameter space.
- Plot the rows of Π as points in parameter space.
- The convex hull of these points has the same boundary structure as the



abstract model.

Transtrum, Mark K. "Manifold boundaries give" gray-box" approximations of complex models." arXiv preprint arXiv:1605.08705 (2016).

REDUCED MODELS OF EXPONENTIAL FAMILIES

The boundary models of the exponential families:

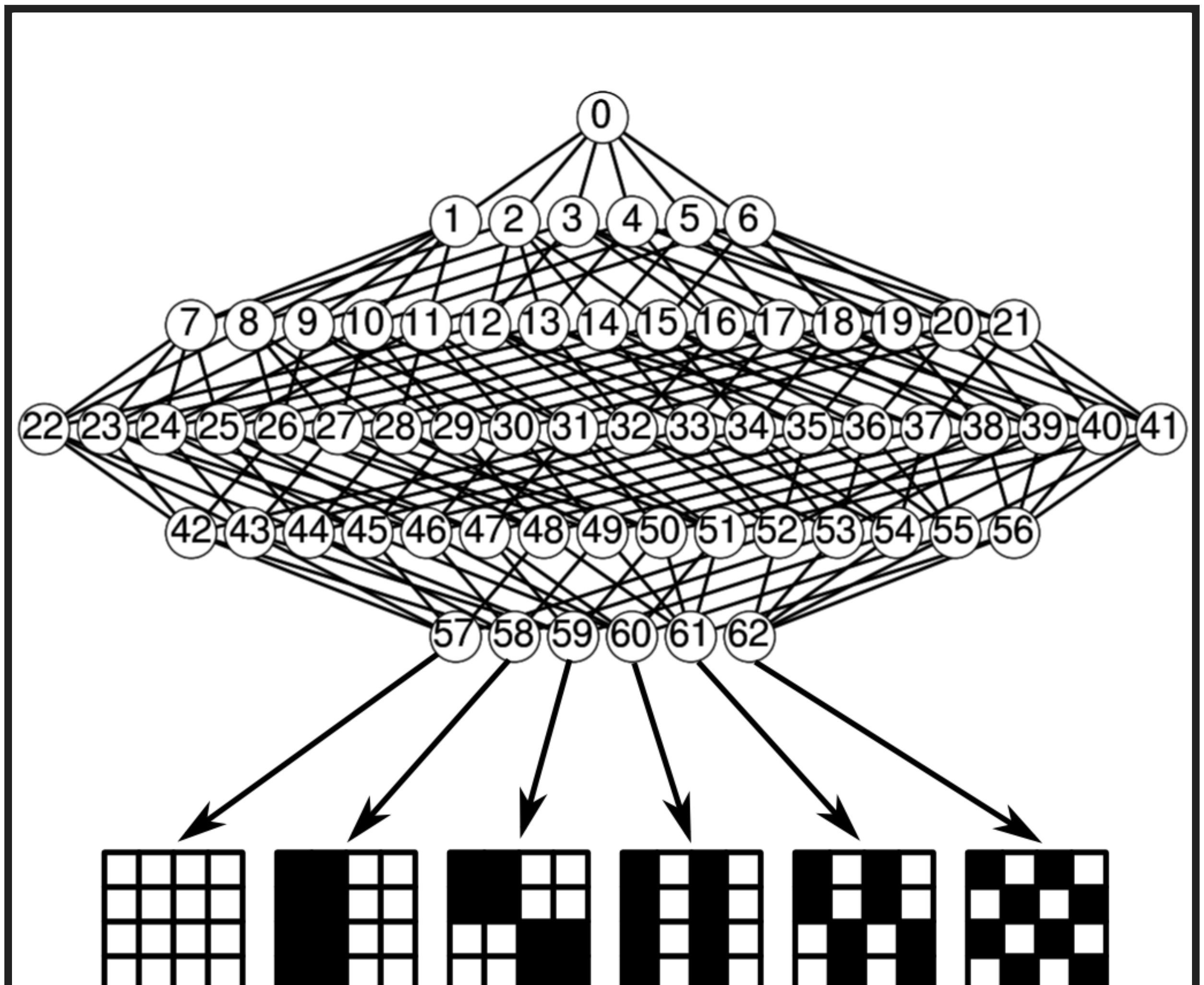
- Several outcomes have zero probability.
- Fewer parameters to describe the relative probabilities among these reduced set of outcomes.

For the case of cluster expansion and crystal structures:

- Zero parameter boundaries have one outcome: the ground state, i.e., stable crystal structure.
- One parameter boundaries describe the control parameter for the phase transition between the two ground states.

EXAMPLE: BINARY ALLOY ON 2D 4X4

UNIT CELL



- Complete information about the phase diagram of this model.
- Which simple models are appropriate for which regimes.

FINAL THOUGHTS ABOUT MODELING COMPLEX SYSTEMS

- There is no theory of complex systems.
- What would a theory look like?
  A theory of using models to confidently make predictions about any scientific question.
  - What model to use?
  - Where is the model valid?
  - Akin to universality classes, RG.

LESSONS FROM INFORMATION

LESSONS FROM INFORMATION TOPOLOGY

- Hasse diagrams are exponentially complex
- Physical systems can exhibit a combinatorially large number of behaviors.
- Most real observations only probe a small set of these behaviors.
- Manifold collapse leads to good approximate models for these limited behaviors.
- Reduced models are only valid for a limited range of behaviors.

- The **Abstract Model Hasse Diagram** relates the intricate description of a complex system through various types of approximations to the set of distinct behavior regimes the model enables.
- The **Observation Semi-Group** relates how different types of coarse-graining lead to systematic compression of the underlying parameter space.

A COMPLEX MODEL MANIFOLD